

4-Hydroxy-1-naphthalenesulfonic acid monosodium salt
6099-57-6 | DTXSID6064113

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 137 °C

Global applicability domain: Inside

Local applicability domain index: 4.28e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>6-Hydroxynaphthalene-2-sulfonic acid</div> <div>Measured: 125</div> <div>Predicted: 128</div>	<div>Image not found</div> <div>Sulisobenzone</div> <div>Measured: 145</div> <div>Predicted: 148</div>	<div>Image not found</div> <div>2-Amino-1-naphthalenesulfonic acid</div> <div>Measured: 180</div> <div>Predicted: 187</div>
<div>Image not found</div> <div>Naphthalene-2-sulfonic acid</div> <div>Measured: 91.0</div> <div>Predicted: 93.1</div>	<div>Image not found</div> <div>Sulindac</div> <div>Measured: 183</div> <div>Predicted: 185</div>	